

Distance and distance signless Laplacian spread of connected graphs *

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Abstract For a connected graph G on n vertices, recall that the distance signless Laplacian matrix of G is defined to be $\mathcal{Q}(G) = Tr(G) + \mathcal{D}(G)$, where $\mathcal{D}(G)$ is the distance matrix, $Tr(G) = diag(D_1, D_2, \dots, D_n)$ and D_i is the row sum of $\mathcal{D}(G)$ corresponding to vertex v_i . Denote by $\rho^{\mathcal{D}}(G)$, $\rho_{min}^{\mathcal{D}}(G)$ the largest eigenvalue and the least eigenvalue of $\mathcal{D}(G)$, respectively. And denote by $q^{\mathcal{D}}(G)$, $q_{min}^{\mathcal{D}}(G)$ the largest eigenvalue and the least eigenvalue of $\mathcal{Q}(G)$, respectively. The distance spread of a graph G is defined as $S_{\mathcal{D}}(G) = \rho^{\mathcal{D}}(G) - \rho_{min}^{\mathcal{D}}(G)$, and the distance signless Laplacian spread of a graph G is defined as $S_{\mathcal{Q}}(G) = q^{\mathcal{D}}(G) - q_{min}^{\mathcal{D}}(G)$. In this paper, we point out an error in the result of Theorem 2.4 in “Distance spectral spread of a graph” [G.L. Yu, et al, Discrete Applied Mathematics. 160 (2012) 2474–2478] and rectify it. As well, we obtain some lower bounds on distance signless Laplacian spread of a graph.

Keywords: Distance matrix; Distance signless Laplacian; Spectral spread

1 Introduction

Throughout this article, we assume that G is a simple, connected and undirected graph on n vertices. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. We denote by $deg(v_i)$ (simply, d_i) the degree of vertex v_i , and for $u, v \in V$, we denote by $d_G(u, v)$ the distance between u and v in G . Recall that the *distance matrix* is $\mathcal{D}(G) = (d_{ij})$ where $d_{ij} = d_G(v_i, v_j)$. For any $v_i \in V(G)$, the *transmission* of vertex v_i , denoted by $Tr_G(v_i)$ or D_i , is defined to be $\sum_{v_j \in V(G), j \neq i} d_G(v_i, v_j)$, which is equal to the row sum of $\mathcal{D}(G)$ corresponding to vertex v_i . Sometimes, D_i is called the *distance degree*. Let $Tr(G) = diag(D_1, D_2, \dots, D_n)$ be the diagonal matrix of vertex transmissions of G . The *distance signless Laplacian matrix* of G is defined as $\mathcal{Q}(G) = Tr(G) + \mathcal{D}(G)$ (see [1]).

For a nonnegative real symmetric matrix M , we denote by $P_M(\lambda) = |\lambda I - M|$ its the characteristic polynomial. Its largest eigenvalue is called the spectral radius of M . For

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a graph G , the *spectral radius* of $\mathcal{D}(G)$ and $\mathcal{Q}(G)$, denoted by $\rho^{\mathcal{D}}(G)$ and $q^{\mathcal{D}}(G)$, are also called the *distance spectral radius* and the *distance signless Laplacian spectral radius*, respectively. Denote by $\rho_{\min}^{\mathcal{D}}(G)$ and $q_{\min}^{\mathcal{D}}(G)$ the least eigenvalue of $\mathcal{D}(G)$ and the least eigenvalue of $\mathcal{Q}(G)$, respectively. The *distance spread* of graph G is defined as $S_{\mathcal{D}}(G) = \rho^{\mathcal{D}}(G) - \rho_{\min}^{\mathcal{D}}(G)$, and the *distance signless Laplacian spread* of graph G is defined as $S_{\mathcal{Q}}(G) = q^{\mathcal{D}}(G) - q_{\min}^{\mathcal{D}}(G)$. Without ambiguity, $S_{\mathcal{D}}(G)$ and $S_{\mathcal{Q}}(G)$ are shortened as $S_{\mathcal{D}}$ and $S_{\mathcal{Q}}$ sometimes.

From [9, 12], we know that the spread of a matrix is a very interesting topic. As a result, in algebraic graph theory, the spread of some matrices of a graph also becomes interesting (see [6], [11]). Because the research of the eigenvalues of the distance matrix of a graph is of great significance for both algebraic graph theory and practical applications, the problem concerning the distance spectrum of a graph has been studied extensively recently (see [5], [3], [7], [2]). These cause the interests of the researchers on the problem about the distance spectral spread of a graph ([14], [10]). Motivated by these, in this paper, we proceed to consider the distance and distance signless Laplacian spread of a graph.

In Section 3, we point out an error in the result of Theorem 2.4 in “Distance spectral spread of a graph” [G.L. Yu, etc, Discrete Applied Mathematics. 160 (2012) 2474–2478] and rectify it. In Section 4, some lower bounds on distance signless Laplacian spread of a graph are obtained.

2 Some preliminaries

In this section, we introduce some definitions, notations and working lemmas.

Let I_p be the $p \times p$ identity matrix and $J_{p,q}$ be the $p \times q$ matrix in which every entry is 1, or simply J_p if $p = q$. For a matrix M , its spectrum $\sigma(M)$ is the multiset of its eigenvalues.

Definition 2.1. Let M be a real matrix of order n described in the following block form

$$M = \begin{pmatrix} M_{11} & \cdots & M_{1t} \\ \vdots & \ddots & \vdots \\ M_{t1} & \cdots & M_{tt} \end{pmatrix}, \quad (2.1)$$

where the diagonal blocks M_{ii} are $n_i \times n_i$ matrices for any $i \in \{1, 2, \dots, t\}$ and $n = n_1 + \dots + n_t$. For any $i, j \in \{1, 2, \dots, t\}$, let b_{ij} denote the average row sum of M_{ij} , i.e. b_{ij} is the sum of all entries in M_{ij} divided by the number of rows. Then $B(M) = (b_{ij})$ (simply by B) is called the *quotient matrix* of M . If in addition for each pair i, j , M_{ij} has constant row sum, then $B(M)$ is called the *equitable quotient matrix* of M .

Consider two sequences of real numbers: $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, and $\mu_1 \geq \mu_2 \geq \dots \geq \mu_m$ with $m < n$. The second sequence is said to *interlace* the first one whenever $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$ for $i = 1, 2, \dots, m$.

Lemma 2.2. ([8]) Let M be a symmetric matrix and have the block form as (2.1), B be the quotient matrix of M . Then the eigenvalues of B interlace the eigenvalues of M .

Lemma 2.3. ([13]) Let M be defined as (2.1), and for any $i, j \in \{1, 2, \dots, t\}$, $M_{ii} = l_i J_{n_i} + p_i I_{n_i}$, $M_{ij} = s_{ij} J_{n_i, n_j}$ for $i \neq j$, where l_i, p_i, s_{ij} are real numbers, $B = B(M)$ be the quotient matrix of M . Then

$$\sigma(M) = \sigma(B) \cup \{p_i^{[n_i-1]} \mid i = 1, 2, \dots, t\}, \quad (2.2)$$

where $\lambda^{[t]}$ means that λ is an eigenvalue with multiplicity t .

By Lemma 2.3, we can obtain the distance (signless Laplacian) spectrum of $K_{a,b}$ as follows immediately, where $n = a + b$.

$$\sigma(\mathcal{D}(K_{a,b})) = \left\{ (-2)^{[n-2]}, n - 2 \pm \sqrt{n^2 - 3ab} \right\}, \quad (2.3)$$

and

$$\sigma(\mathcal{Q}(K_{a,b})) = \left\{ (2n - a - 4)^{[b-1]}, (2n - b - 4)^{[a-1]}, \frac{5n - 8 \pm \sqrt{9n^2 - 32ab}}{2} \right\}. \quad (2.4)$$

Lemma 2.4. ([4]) *Let H_n denote the set of all $n \times n$ Hermitian matrices, $A \in H_n$ with eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, and B be a $m \times m$ principal matrix of A with eigenvalues $\mu_1 \geq \mu_2 \geq \dots \geq \mu_m$. Then $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$ for $i = 1, 2, \dots, m$.*

3 Results on $S_{\mathcal{D}}$ for a bipartite graph

In [14], the authors obtained a lower bound for $S_{\mathcal{D}}(G)$ with the maximum degree Δ of G , but it is found that the result is incorrect when $\Delta \leq |V(G)| - 2$. In this section, we rectify it.

Let $G = (V, E)$ be a graph. For $v_i, v_j \in V$, if v_i is adjacent to v_j , we denote it by $v_i \sim v_j$ (simply, $i \sim j$). We let $t_v = \frac{\sum_{v_i \sim v} D_i}{d_v}$ be the *average distance degree* of v ([14]).

Proposition 3.1. ([14], Theorem 2.4) *Let G be a simple connected bipartite graph on n vertices with $S = \sum_{i=1}^n D_i$ and maximum degree Δ . Suppose $\deg(v_1) = \deg(v_2) = \dots = \deg(v_k) = \Delta$. Then*

(i) *if $\Delta \leq n - 2$, we have*

$$S_{\mathcal{D}}(G) \geq \max_{1 \leq i \leq k} \frac{\sqrt{a_i^2 - 4b_i(\Delta + 1)(n - \Delta - 1)}}{(\Delta + 1)(n - \Delta - 1)}, \quad (3.1)$$

where $a_i = 2(n - t_{v_i} - 1)\Delta^2 + (S - 2t_{v_i} - 2)\Delta + S$ and $b_i = \Delta^2(2S - t_{v_i}^2 - 2t_{v_i} - 1)$.

(ii) *if $\Delta = n - 1$, we have*

$$S_{\mathcal{D}}(G) = \begin{cases} 0, & \text{if } n = 1; \\ 2, & \text{if } n = 2; \\ n + \sqrt{n^2 - 3n + 3}, & \text{if } n \geq 3. \end{cases}$$

Let $N(v_i) = \{v_{i_1}, v_{i_2}, \dots, v_{i_{\Delta}}\}$ be the neighbors set of v_i , and $N[v_i] = N(v_i) \cup \{v_i\}$. In the proof of (3.1), the authors partition $V(G)$ into two parts $N[v_i]$ and $V(G) \setminus N[v_i]$ for some $1 \leq i \leq k$. Corresponding to this partition, $\mathcal{D}(G)$ can be written as

$$\mathcal{D}(G) = \begin{pmatrix} 0 & 1 & 1 & \dots & 1 & \\ 1 & 0 & 2 & \dots & 2 & * \\ 1 & 2 & 0 & \dots & 2 & \\ \dots & \dots & \dots & \dots & \dots & \\ 1 & 2 & 2 & \dots & 0 & * \\ & & * & & & * \end{pmatrix}. \quad (3.2)$$

Then the author presented the quotient matrix of $\mathcal{D}(G)$ as:

$$B_1 = \begin{pmatrix} \frac{2\Delta^2}{\Delta+1} & \frac{t_{v_i}\Delta+\Delta-2\Delta^2}{\Delta+1} \\ \frac{t_{v_i}\Delta+\Delta-2\Delta^2}{n-\Delta-1} & \frac{S-2t_{v_i}\Delta+2\Delta(\Delta-1)}{n-\Delta-1} \end{pmatrix}. \quad (3.3)$$

The following example shows that (3.3) is false.

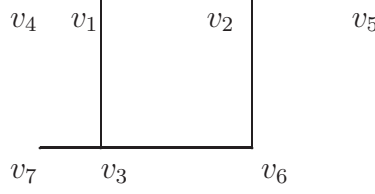


Fig. 3.1. G_1

For the above graph (see Fig. 3.1), it is clear that $\Delta = 3, t_{v_1} = \frac{34}{3}, S = 84$ and

$$\mathcal{D}(G) = (d_{ij})_{7 \times 7} = \left(\begin{array}{cccc|ccc} 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 1 & 0 & 2 & 2 & 1 & 1 & 3 \\ 1 & 2 & 0 & 2 & 3 & 1 & 1 \\ 1 & 2 & 2 & 0 & 3 & 3 & 3 \\ \hline 2 & 1 & 3 & 3 & 0 & 2 & 4 \\ 2 & 1 & 1 & 3 & 2 & 0 & 2 \\ 2 & 3 & 1 & 3 & 4 & 2 & 0 \end{array} \right), \quad (3.4)$$

and by (3.3), we have the quotient matrix $B_1 = \begin{pmatrix} \frac{18}{4} & \frac{19}{4} \\ \frac{19}{3} & \frac{4}{3} \end{pmatrix}$. In fact the quotient matrix can be computed by the definition of the quotient matrix and (3.4) immediately as $B_2 = \begin{pmatrix} \frac{18}{4} & \frac{25}{4} \\ \frac{4}{25} & \frac{16}{3} \end{pmatrix} \neq B_1$, it is a contradiction.

Noticing the error in (3.3), with the similar technique, we rectify (3.1) as follows.

Theorem 3.2. *Let G be a simple connected bipartite graph on n vertices, Δ be the maximum degree of G , $S = \sum_{i=1}^n D_i$. Suppose that $\deg(v_1) = \deg(v_2) = \dots = \deg(v_k) = \Delta \leq n-2$ for some k ($1 \leq k \leq n$). Then*

$$S_{\mathcal{D}}(G) \geq \max_{1 \leq i \leq k} \frac{\sqrt{a_i^2 + 4b_i(1+\Delta)(n-\Delta-1)}}{(1+\Delta)(n-\Delta-1)}, \quad (3.5)$$

where $a_i = (\Delta+1)(S-2D_i-2t_{v_i}\Delta) + 2n\Delta^2$ and $b_i = D_i^2 - 2S\Delta^2 + 2D_it_{v_i}\Delta + t_{v_i}^2\Delta^2$.

Proof. $V(G)$ is partitioned into two parts which are $N[v_i]$ and $V(G) \setminus N[v_i]$ for some $1 \leq i \leq k$. Corresponding to this partition, $\mathcal{D}(G)$ is written as (3.2) and the quotient matrix B of $\mathcal{D}(G)$ is presented as follow:

$$B = \begin{pmatrix} \frac{2\Delta^2}{\Delta+1} & \frac{t_{v_i}\Delta+D_i-2\Delta^2}{\Delta+1} \\ \frac{t_{v_i}\Delta+D_i-2\Delta^2}{n-\Delta-1} & \frac{S-2t_{v_i}\Delta+2\Delta^2-2D_i}{n-\Delta-1} \end{pmatrix}.$$

Then

$$P_B(\lambda) = |\lambda I - B| = \lambda^2 - \frac{(\Delta+1)(S-2D_i-2t_{v_i}\Delta)+2n\Delta^2}{(1+\Delta)(n-\Delta-1)}\lambda - \frac{D_i^2-2S\Delta^2+2D_it_{v_i}\Delta+t_{v_i}^2\Delta^2}{(1+\Delta)(n-\Delta-1)}.$$

Let $P_B(\lambda) = 0$. It follows that

$$\lambda_{1,2} = \frac{a_i \pm \sqrt{a_i^2 + 4b_i(1 + \Delta)(n - \Delta - 1)}}{2(1 + \Delta)(n - \Delta - 1)},$$

where $a_i = (\Delta + 1)(S - 2D_i - 2t_{v_i}\Delta) + 2n\Delta^2$ and $b_i = D_i^2 - 2S\Delta^2 + 2D_it_{v_i}\Delta + t_{v_i}^2\Delta^2$. Using Lemma 2.2 gets (3.5). \square

Remark 3.1

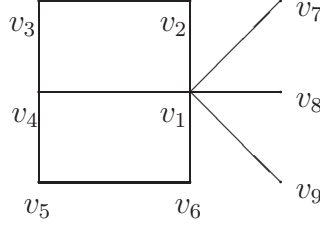


Fig. 3.2. G_2

graph	Theorem 3.2	approximate value
G_1	$S_{\mathcal{D}}(G) \geq 15.5960$	$S_{\mathcal{D}}(G) \approx 17.6820$
G_2	$S_{\mathcal{D}}(G) \geq 19.0059$	$S_{\mathcal{D}}(G) \approx 20.9674$

Table 3.1.

By computation with mathematica for graphs G_1 and G_2 (see Figs. 3.1, 3.2 and Table 3.1), it seems that Theorems 3.2 is useful to evaluate the distance spread of a bipartite graph.

From the proof of Theorem 3.2 and by Lemma 2.2, we have the following corollary immediately.

Corollary 3.3. *Let G be a simple connected bipartite graph on $n \geq 3$ vertices with maximum degree $\Delta \leq n - 2$. Suppose that $\deg(v_1) = \deg(v_2) = \dots = \deg(v_k) = \Delta$, a_i, b_i are defined as Theorem 3.2 for $1 \leq i \leq k$. Then*

- (i) $\rho^{\mathcal{D}}(G) \geq \max_{1 \leq i \leq k} \frac{a_i + \sqrt{a_i^2 + 4b_i(1 + \Delta)(n - \Delta - 1)}}{2(1 + \Delta)(n - \Delta - 1)};$
- (ii) $\rho_{min}^{\mathcal{D}}(G) \leq \min_{1 \leq i \leq k} \frac{a_i + \sqrt{a_i^2 + 4b_i(1 + \Delta)(n - \Delta - 1)}}{2(1 + \Delta)(n - \Delta - 1)}.$

4 On $S_{\mathcal{Q}}$

In this section, we show some bounds of $S_{\mathcal{Q}}$ for bipartite graphs and some bounds with some parameters.

4.1 Bounds on $S_{\mathcal{Q}}$ for bipartite graphs

For a graph G , $W(G) = \sum_{1 \leq i < j \leq n} d_{ij}$ is called *Wiener index*. Thus, $W(G) = \frac{1}{2} \sum_{i=1}^n D_i$ and $S = 2W(G)$. Similar to the proof of Theorem 3.2 and Corollary 3.3, we get the following theorem and one corollary in term of *Wiener index*.

Theorem 4.1. Let G be a simple connected bipartite graph on $n \geq 3$ vertices with maximum degree Δ and Wiener index W . Suppose that $\deg(v_1) = \deg(v_2) = \dots = \deg(v_k) = \Delta$. Then
(i) if $\Delta \leq n - 2$, then

$$S_{\mathcal{Q}}(G) \geq \max_{1 \leq i \leq k} \frac{\sqrt{a_i^2 + 4b_i(1 + \Delta)(n - \Delta - 1)}}{(1 + \Delta)(n - \Delta - 1)}, \quad (4.1)$$

where $a_i = 4(W - D_i - t_{v_i}\Delta)(\Delta + 1) + 2n\Delta^2 + nD_i + nt_{v_i}\Delta$ and $b_i = 4D_i^2 + 8D_it_{v_i}\Delta + 4t_{v_i}^2\Delta^2 - 8W\Delta^2 - 4WD_i - 4Wt_{v_i}\Delta$.

(ii) if $\Delta = n - 1$, then $S_{\mathcal{Q}}(G) = \sqrt{9n^2 - 32n + 32}$.

Remark 4.1

graph	Theorem 4.1	approximate value
G_1	$S_{\mathcal{Q}}(G) \geq 15.6400$	$S_{\mathcal{Q}}(G) \approx 18.6100$
G_2	$S_{\mathcal{Q}}(G) \geq 17.8520$	$S_{\mathcal{Q}}(G) \approx 21.1870$

Table 4.1.

By computation with mathematica for graphs G_1 and G_2 (see Figs. 3.1, 3.2 and Table 4.1), it seems that Theorem 4.1 is useful to evaluate the signless Laplacian distance spread of a bipartite graph.

Corollary 4.2. Let G be a simple connected bipartite graph on $n \geq 3$ vertices, $\Delta \leq n - 2$ be maximum degree of G . Suppose that $\deg(v_1) = \deg(v_2) = \dots = \deg(v_k) = \Delta$ for some k ($1 \leq k \leq n$), a_i, b_i are defined as Theorem 4.1 for $1 \leq i \leq k$. Then

$$(i) \quad q^{\mathcal{D}}(G) \geq \max_{1 \leq i \leq k} \frac{a_i + \sqrt{a_i^2 + 4b_i(1 + \Delta)(n - \Delta - 1)}}{2(1 + \Delta)(n - \Delta - 1)};$$

$$(ii) \quad q_{\min}^{\mathcal{D}}(G) \leq \min_{1 \leq i \leq k} \frac{a_i + \sqrt{a_i^2 + 4b_i(1 + \Delta)(n - \Delta - 1)}}{2(1 + \Delta)(n - \Delta - 1)}.$$

Lemma 4.3. Let $n \geq 4$ and a be positive integers with $2a \leq n$. Then $S_{\mathcal{Q}}(K_{a, n-a}) \geq S_{\mathcal{Q}}(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil})$ with equality if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

Proof. By (2.4), we have

$$\sigma(\mathcal{Q}(K_{a, n-a})) = \left\{ (2n - a - 4)^{[n-a-1]}, (n + a - 4)^{[a-1]}, \frac{5n - 8 \pm \sqrt{9n^2 - 32a(n-a)}}{2} \right\}.$$

It is checked that

$$\frac{5n - 8 + \sqrt{9n^2 - 32a(n-a)}}{2} > 2n - a - 4, \quad \frac{5n - 8 - \sqrt{9n^2 - 32a(n-a)}}{2} > n + a - 4.$$

Then $q^{\mathcal{D}}(K_{a, n-a}) = \frac{5n-8+\sqrt{9n^2-32a(n-a)}}{2}$, and

$$q_{\min}^{\mathcal{D}}(K_{a, n-a}) = \begin{cases} n + a - 4, & a > 1 \\ \frac{5n-8-\sqrt{9n^2-32a(n-a)}}{2}, & a = 1. \end{cases}$$

When $0 < a \leq \frac{n}{2}$, it checked that $f(a) = \frac{5n-8+\sqrt{9n^2-32a(n-a)}}{2}$ is a decreasing function with respect to a , $g(a) = n + a - 4$ is a increasing function with respect to a . Then we have $S_{\mathcal{Q}}(K_{2, n-2}) > S_{\mathcal{Q}}(K_{3, n-3}) > \dots > S_{\mathcal{Q}}(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil})$.

Noting that $n \geq 4$, by directly computation, we have

$$S_Q(K_{1,n-1}) - S_Q(K_{2,n-2})$$

$$= \sqrt{9n^2 - 32n + 32} - \left(\frac{5n - 8 + \sqrt{9n^2 - 64n + 128}}{2} - (n - 2) \right) > 0.$$

Thus $S_Q(K_{1,n-1}) > S_Q(K_{2,n-2}) > S_Q(K_{3,n-3}) > \dots > S_Q(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil})$. This completes the proof. \square

Let G be a simple connected bipartite graph on n vertices. If $n = 4$, G is isomorphic to one of the following three graphs: (1) $K_{2,2}$, (2) P_4 , (3) S_4 ; if $n = 5$, G is isomorphic to one of the following five graphs: (4) $K_{2,3}$, (5) G_5 , (6) G_6 , (7) P_5 , (8) S_5 (see Fig. 4.1).

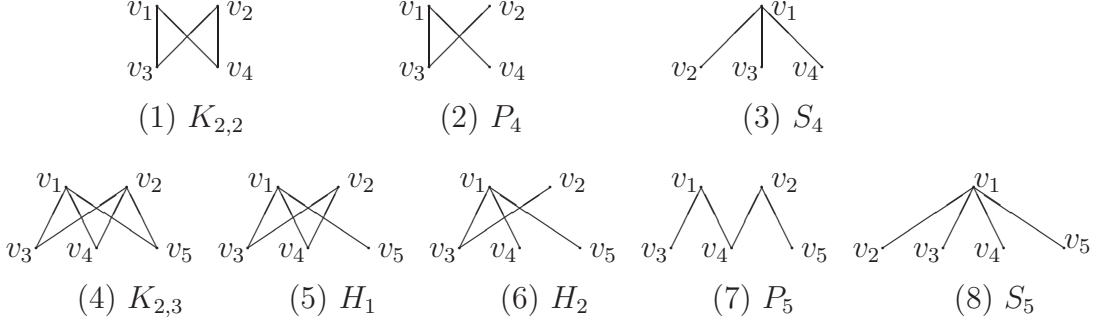


Fig. 4.1. $K_{2,2}$ - S_5

By direct calculation, we obtain the following two tables.

G	$q^{\mathcal{D}}$	$q_{min}^{\mathcal{D}}$	$S_Q(G)$
$K_{2,2}$	8	2	6
P_4	10.6056	2	8.6056
S_4	9.4641	2.5359	6.9282

Table 4.1

G	$q^{\mathcal{D}}$	$q_{min}^{\mathcal{D}}$	$S_Q(G)$
$K_{2,3}$	11.3723	3	8.3723
H_1	13.3441	3.3113	10.0328
H_2	15.3119	3.6075	11.7044
P_5	17.1152	3.4385	13.6767
S_5	13.4244	3.5756	9.8488

Table 4.2

Combining Lemma 4.3 and the results in Table 4.1, we get the following corollary.

Corollary 4.4. *For positive integers n and a with $2a \leq n$, $S_Q(K_{a,n-a}) \geq S_Q(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil})$ with equality if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.*

Comparing the results in Tables 4.1 and 4.2, and checking more graphs with computer, it seems that among bipartite graphs, $S_Q(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil})$ always has the minimum S_Q . Thus, we propose the following problem for further research.

Conjecture 4.5. *Let G be a bipartite graph with n vertices. Then $S_Q(G) \geq S_Q(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil})$ with equality if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.*

Remark 4.2 In order to prove Conjecture 4.5, maybe it is better to show $S_Q(G) \geq S_Q(K_{a,n-a})$ holding for some a at first, and then to using Lemma 4.3 to get the desired result.

4.2 Bound on S_Q with clique number

A *clique* of a graph G is a subgraph in which any pair of vertices is adjacent, and the clique number $\omega(G)$ (simply, ω) is the number of vertices of the largest clique in G . In this subsection, we present a lower bound on S_Q with clique number.

Theorem 4.6. *Let G be a simple connected graph with n vertices, clique number $\omega \geq 2$ and Wiener index W . Suppose that G_1, G_2, \dots, G_k are all the cliques with order ω , $s_i = \sum_{v_j \in V(G_i)} D_j$ for $1 \leq i \leq k$. Then*

- (i) *if $\omega = n$, then $S_Q(G) = n$;*
- (ii) *if $2 \leq \omega \leq n - 1$, then*

$$S_Q(G) \geq \max_{1 \leq i \leq k} \frac{\sqrt{a_i^2 - 4b_i(n - \omega)\omega}}{(n - \omega)\omega}, \quad (4.2)$$

where $a_i = n\omega(1 - \omega) + 4\omega(s_i - W) - ns_i$ and $b_i = 4W\omega(\omega - 1) + 4s_i(W - s_i)$.

Proof. (i). If $\omega = n$, then $G \cong K_n$. By direct calculation, we have $q^D(G) = 2n - 2$ and $q_{min}^D(G) = n - 2$. Thus $S_D(G) = q^D(G) - q_{min}^D(G) = n$.

(ii). If $\omega \leq n - 1$, for $1 \leq i \leq k$, suppose $V(G_i) = \{v_{i1}, v_{i2}, \dots, v_{i\omega}\}$. Then $V(G)$ is divided into two parts $V(G_i)$ and $V(G) \setminus V(G_i)$. Corresponding to this partition, the quotient matrix of $Q(G)$ is written as

$$B = \begin{pmatrix} \frac{\omega(\omega-1)+s_i}{\omega} & \frac{s_i-\omega(\omega-1)}{\omega} \\ \frac{s_i-\omega(\omega-1)}{n-\omega} & \frac{4W-3s_i+\omega(\omega-1)}{n-\omega} \end{pmatrix}.$$

Similar to the proof of Theorem 3.2, solving $P_B(\lambda) = 0$ and using Lemma 2.2 get (4.2). \square

Remark 4.3 Recall that a kite $Ki_{n,\omega}$ is the graph obtained from a clique K_ω and a path $P_{n-\omega}$ by adding an edge between an endpoint of the path and a vertex of the clique. For a kite $G = Ki_{5,3}$, by Theorem 4.6, we have $S_Q(G) \geq 10.6158$. On the other hand, by direct calculation, we obtain $S_Q(G) \approx 11.3395$. This shows that Theorem 4.6 is useful to evaluate the distance signless Laplacian spread of a graph with given clique number.

By Lemma 2.2 and Theorem 4.6, we have

Corollary 4.7. *Let G be a simple connected graph with n vertices and clique number ω . Suppose that G_1, G_2, \dots, G_k are all the cliques with order ω , a_i, b_i are defined as Theorem 4.6 for $1 \leq i \leq k$. Then*

- (i) $q^D(G) \geq \max_{1 \leq i \leq k} \left\{ \frac{-a_i + \sqrt{a_i^2 - 4b_i(n - \omega)\omega}}{2(n - \omega)\omega} \right\};$
- (ii) $q_{min}^D(G) \leq \min_{1 \leq i \leq k} \left\{ \frac{-a_i - \sqrt{a_i^2 - 4b_i(n - \omega)\omega}}{2(n - \omega)\omega} \right\}.$

4.3 Bound on S_Q with diameter

In this subsection, we obtain a lower bound on S_Q of a graph with diameter. In a graph, a path is called a diameter path if its length is equal to the diameter of this graph.

Theorem 4.8. *Let G be a simple connected graph with n vertices, diameter d and Wiener index W . Suppose that P_1, P_2, \dots, P_k are all the diameter paths, and suppose that $s_i = \sum_{v_j \in V(P_i)} D_j$ for $1 \leq i \leq k$. Then*

- (i) if $d = 1$, then $S_Q(G) = n$;
(ii) if $2 \leq d$, then

$$S_Q(G) \geq \max_{1 \leq i \leq k} \frac{\sqrt{a_i^2 - 12b_i(d+1)(n-1-d)}}{3(d+1)(n-1-d)}, \quad (4.3)$$

where $a_i = 12(1+d)(s_i - W) - nd(d+1)(d+2) - 3ns_i$ and $b_i = 4d(d+1)(d+2)W + 12s_i(W - s_i)$.

Proof. (i). If $d = 1$, then $G \cong K_n$. By direct calculation, $q^D(G) = 2n - 2$, $q_{min}^D(G) = n - 2$. Thus, $S_D(G) = n$.

(ii). If $2 \leq d$, for $1 \leq i \leq k$, we let $T = \sum_{v_s, v_j \in V(P_i)} d_{sj}$. Then when d is even, we have

$$\begin{aligned} T &= 2(1 + 2 + \dots + d) + 2[1 + 1 + 2 + 3 + \dots + (d-1)] + \dots \\ &\quad + 2[1 + 1 + 2 + 2 + \dots + (\frac{d}{2} - 1) + (\frac{d}{2} - 1) + \frac{d}{2} + (\frac{d}{2} + 1)] \\ &\quad + 2[1 + 2 + \dots + (\frac{d}{2} - 1) + \frac{d}{2}], \\ &= d(d+1) + [(d-1)d + 2 \times 1] + [(d-2)(d-1) + 2 \times 3] + \dots \\ &\quad + [(\frac{d}{2} + 1)(\frac{d}{2} + 2) + (\frac{d}{2} - 1)\frac{d}{2}] + \frac{d}{2}(\frac{d}{2} + 1) \\ &= 1^2 + 2^2 + 3^2 + \dots + d^2 + 1 + 2 + 3 + \dots + d \\ &= \frac{d(d+1)(d+2)}{3}. \end{aligned}$$

When d is odd, we have

$$\begin{aligned} T &= 2(1 + 2 + \dots + d) + 2[1 + 1 + 2 + 3 + \dots + (d-1)] + \dots \\ &\quad + 2(1 + 1 + 2 + 2 + \dots + \frac{d-1}{2} + \frac{d-1}{2} + \frac{d+1}{2}) \\ &= d(d+1) + [(d-1)d + 2 \times 1] + [(d-2)(d-1) + 2 \times 3] + \dots \\ &\quad + (\frac{d+1}{2})(\frac{d+1}{2} + 1) + (\frac{d-1}{2})(\frac{d-1}{2} + 1) \\ &= 1^2 + 2^2 + 3^2 + \dots + d^2 + 1 + 2 + 3 + \dots + d \\ &= \frac{d(d+1)(d+2)}{3}. \end{aligned}$$

Now $V(G)$ is partitioned into two parts which are $V(P_i)$ and $V(G) \setminus V(P_i)$. Corresponding to this partition, the quotient matrix of $Q(G)$ can be written as

$$B = \begin{pmatrix} \frac{\frac{1}{3}d(d+1)(d+2)+s_i}{d+1} & \frac{s_i - \frac{1}{3}d(d+1)(d+2)}{d+1} \\ \frac{s_i - \frac{1}{3}d(d+1)(d+2)}{n-d-1} & \frac{4W - 3s_i + \frac{1}{3}d(d+1)(d+2)}{n-d-1} \end{pmatrix}.$$

Similar to the proof of Theorem 3.2, solving $P_B(\lambda) = 0$ and using Lemma 2.2 get (4.3). \square

Remark 4.4 For G_1 shown in Fig. 3.1, then by Theorem 4.8, we have $S_Q(G) \geq 12.1198$. From the Table 4.1, we know that $S_Q(G_1) \approx 18.6100$. This shows that Theorem 4.8 is useful to evaluate the distance signless Laplacian spread of a graph with given diameter.

Corollary 4.9. Let G be a simple connected graph with n vertices and diameter d . Suppose that the path P_1, P_2, \dots, P_k are all the diameter of G , a_i, b_i are defined as Theorem 4.8 for $1 \leq i \leq k$. Then

- (i) $q^D(G) \geq \max_{1 \leq i \leq k} \left\{ \frac{-a_i + \sqrt{a_i^2 - 12b_i(d+1)(n-1-d)}}{6(d+1)(n-1-d)} \right\};$
(ii) $q_{min}^D(G) \leq \min_{1 \leq i \leq k} \left\{ \frac{-a_i - \sqrt{a_i^2 - 12b_i(d+1)(n-1-d)}}{6(d+1)(n-1-d)} \right\}.$

4.4 Bound On S_Q for cacti with given circumference

A connected graph G is a *cactus* if any two of its cycles have at most one common vertex. *Circumference* is the length of the longest cycle of a graph. In this section, we present a lower bound on S_Q of a cactus with given circumference.

Theorem 4.10. *Let G be a cactus on n vertices with circumference l ($l \geq 3$) and Wiener index W . Suppose that cycles C_1, C_2, \dots, C_k are all with length l , $s_i = \sum_{v_j \in V(C_i)} D_j$ for $1 \leq i \leq k$. Then*

$$S_Q(G) \geq \max_{1 \leq i \leq k} \frac{\sqrt{a_i^2 - 16b_i l(n-l)}}{4l(n-l)}, \quad (4.4)$$

where

$$a_i = \begin{cases} l^3 n + 4ns_i - 16l(s_i - W), & \text{if } l \text{ is even;} \\ l^3 n + 4ns_i - ln - 16l(s_i - W), & \text{if } l \text{ is odd,} \end{cases}$$

and

$$b_i = \begin{cases} 4l^3 W - 16s_i(s_i - W), & \text{if } l \text{ is even;} \\ 4(l^3 - l)W - 16s_i(s_i - W), & \text{if } l \text{ is odd,} \end{cases}$$

Proof. Corresponding to C_i , $V(G)$ is partitioned into two parts $V(C_i)$ and $V(G) \setminus V(C_i)$.

Case 1: l is even.

Then for any $v \in V(C_i)$, the sum of distance from vertex v to all other vertices on cycle $V(C_i)$ is $\frac{l^2}{4}$. Corresponding to the above partition, the quotient matrix of $\mathcal{Q}(G)$ is written as

$$B = \begin{pmatrix} \frac{l^2}{4} + \frac{S_i}{l} & \frac{S_i}{l} - \frac{l^2}{4} \\ \frac{S_i - \frac{l^3}{4}}{n-l} & \frac{4W - 3S_i + \frac{l^3}{4}}{n-l} \end{pmatrix}.$$

Similar to the proof of Theorem 3.2, solving $P_B(\lambda) = 0$ and using Lemma 2.2 get (4.2).

Case 2: l is odd.

Then for any $v \in V(C_i)$, the sum of distance from vertex v to all other vertices on cycle $V(C_i)$ is $\frac{l^2-1}{4}$. Corresponding to the above partition, the quotient matrix of $\mathcal{Q}(G)$ is written as

$$B = \begin{pmatrix} \frac{l^2-1}{4} + \frac{S_i}{l} & \frac{S_i}{l} - \frac{l^2-1}{4} \\ \frac{S_i - \frac{l^3-1}{4}}{n-l} & \frac{4W - 3S_i + \frac{l^3-1}{4}}{n-l} \end{pmatrix}.$$

Similar to the proof of Theorem 3.2, solving $P_B(\lambda) = 0$ and using Lemma 2.2 get (4.2). \square

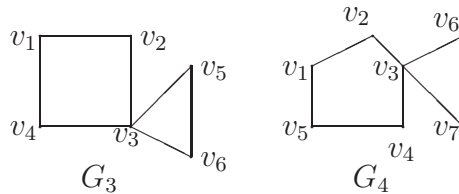


Fig. 4.2. G_3, G_4

Remark 4.4 Let G_3, G_4 are as shown in Fig. 4.2. By Theorem 4.10, we have $s_Q(G_3) \geq 11.5$. On the other hand, by direct calculation, we have $S_Q(G_3) \approx 12.8$. By Theorem 4.10, we have $S_Q(G_4) \geq 13.4$. On the other hand, by direct calculation, we have $S_Q(G_4) \approx 16.3$. These two examples show that Theorem 4.10 is useful to evaluate the S_Q of the cacti with given circumference.

Corollary 4.11. *Let G be a cactus on n vertices with given circumference $l \geq 3$. Suppose that cycles C_1, C_2, \dots, C_k are all with length l , a_i, b_i are defined as Theorem 4.10 for $1 \leq i \leq k$. Then*

$$(1) \ q^{\mathcal{D}}(G) \geq \max_{1 \leq i \leq k} \left\{ \frac{-a_i + \sqrt{a_i^2 - 16b_i l(n-l)}}{8l(n-l)} \right\};$$

$$(2) \ q_{min}^{\mathcal{D}}(G) \leq \min_{1 \leq i \leq k} \left\{ \frac{-a_i - \sqrt{a_i^2 - 16b_i l(n-l)}}{8l(n-l)} \right\}.$$

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